02/01/2019 Geometrical band theory and topological insulators.

4 lectures of 1,5 hours.

I. Homotopy groups & fiber bundles } background material in topology & geometry
(topological defects) (Dirac monopole) in order to have a common language

II. Geometrical band theory and (Berry phases in solid state physics) } core/heart of the subject

III. TRB topological insulators : QHE and the Haldane model
($\mathbb{Z}$)

IV. TRS topological insulator : Kane & Mele's model } two concrete examples
($\mathbb{Z}_2$)

General introduction :
(Main message)
band theory is richer than previously thought

1) Modern band theory : band theory is not only about energy bands $E_n(\vec{k})$
but also about Bloch functions $u_n(\vec{k})$ i.e. wavefunctions.
some physical quantities depend on the phase of $u_n(\vec{k})$

{ hidden geometrical structure in band theory due to coupling between bands
{ emergent static gauge field : Berry phases
also quantum metric

↳ also called fiber bundle

→ geometry : local properties in $\vec{k}$ space . Anomalous velocity.

→ topology : global ——— . Quantum Hall effect.

2) Topological insulator : similar to the quantum Hall effect in at least three respects :
- bulk insulator (characterized by an integer invariant)
- conducting edge states that are robust (chiral or helical or ...)
- bulk-edge correspondance : # of chiral edge modes
= change in topological invariant across the boundary

(a trivial insulator is adiabatically connected to an atomic insulator)

3) Dirac in condensed matter

a) Dirac equation : emergent
as the minimal band coupling
quantum mechanical
also Jackiw-Rebbi

b) Projection in an adiabatic/semiclassical limit [e.g. Dirac eqt in 3+1 to Pauli eqt]
emergent gauge field/fiber bundle [e.g. Dirac magnetic monopole]
also Aharonov-Bohm, Berry

I. Topological defects and the Dirac monopole

During the first lecture we will review background material needed to describe geometrical/topological band theory.

These are mathematical notions but we will use physical examples to introduce them.

A first example is homotopy groups (a notion of topology introduced by Poincaré 1895), which we will introduce via topological defects in order parameters.

A second example is fiber bundles (a notion of geometry developped by Whitney, Stiefel, Pontryagin & Chern 30's-40's), which we will review via the magnetic monopole of Dirac 1931.

1) Topological defects in order parameters

original works by Kleman, Toulouse, Mineev, Volovik, Mermin 1976-79
nice review by James Sethna 1991 on his website

In the realm of Landau's theory of phase transitions. In his view, different phases of matter are distinguished by different symmetries and are characterized by an order parameter (O.P.). Sethna describes Landau's theory as a four-step procedure:

1. Identify the broken symmetry
2. Define an O.P.
3. Study the elementary linear excitations (small oscillations of the O.P.)
4. Classify the topological defects of the O.P.

A topological defect is a singularity of the O.P. that can not be patched/repaired by any local rearrangement.

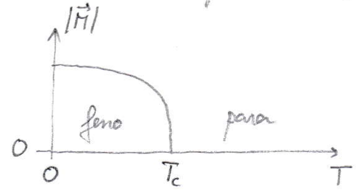
number of components of the O.P.

ex: Heisenberg ($n=3$) ferromagnet in 3D ($d=3$)

broken symmetry = $\begin{cases} \text{space rotations } SO(3) \longrightarrow SO(2) \\ \text{time-reversal (TR)} \end{cases}$ [we are left with rotations around the magnetization direction]

O.P. = local magnetization $\vec{M}(\vec{r})$

In the ordered phase, at low temperature ($T \ll T_c$), the norm of the magnetizat° is almost constant



Therefore $\vec{M}(\vec{r}) \simeq M_0\, \vec{n}(\vec{r})$ $\in S^2$ (ie. usual sphere)

Because there is a SSB of a continuous symmetry $SO(3) \xrightarrow{SSB} SO(2)$, soft modes appear (Goldstone). There are two transverse spin waves.

What about topological defects?

To capture a d'-dim. defect ($d'=0$ is a point, $d'=1$ is a line, $d'=2$ is a plane) one needs a r-dim. cage such that

$$\boxed{1+d'+r=d}$$

which is the hunter's rule (Kleman & Toulouse)

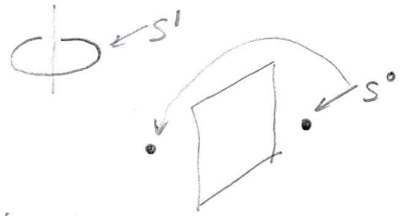
For example, in $d=3$ a point-like defect $d'=1$ require a $r=2$-dim cage.

One therefore tries to classify inequivalent maps from

$$\begin{array}{ccc} \text{cage in physical space} & \longrightarrow & \text{O.P. space} = V \\ S^2 & & S^2 \\ \vec{r} & \longmapsto & \vec{n}(\vec{r}) \end{array}$$

For a line-like defect, maps $S^1 \longrightarrow S^2$

For a plane-like defect, maps $S^0 \longrightarrow S^2$



Mathematicians came to the rescue with the notion of homotopy groups (Poincaré 1895, Analysis situs).

We look for equivalence classes of oriented loops (S^1) drawn on manifolds. This will allow us to classify maps. We are allowed to continuously deform the loops but not to cut or glue.

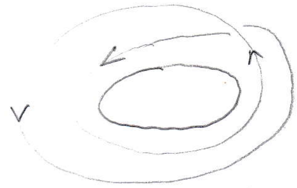
examples:

- $S^1 \longrightarrow S^1$ circle

  $\Pi_1(S^1) = \mathbb{Z}$ ie the group $\{\mathbb{Z}; +\}$

  ↑ 1st homotopy group (fundamental group)

  there are as many classes as elements in $\mathbb{Z}$



winding number = +2

$W \in \mathbb{Z}$

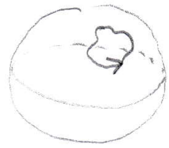
$\underbrace{\qquad\qquad}_{\text{first example of a topological invariant}}$

- $S^1 \longrightarrow S^2$ sphere

  $\Pi_1(S^2) = 0$ ie the trivial group $\{0; +\}$

  There is a single trivial class

  "One cannot lasso a basketball."



There is no winding #

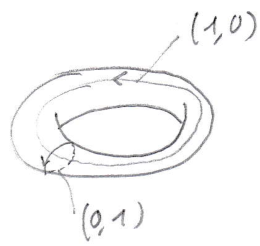
- $S^1 \longrightarrow T^2 = S^1 \times S^1$ torus

  $\Pi_1(T^2) = \mathbb{Z} \times \mathbb{Z}$

  There are two types of non-contractible loops

  one needs ~~two~~ integers

  The topological invariant here is (W_1, W_2)



- One can generalize the notion to manifolds other than S^1

  $S^2 \longrightarrow S^2$

  $\Pi_2(S^2) = \mathbb{Z}$ mapping number

  ↑ 2nd homotopy group

- By convention $\Pi_0(V)$ gives the number of connex components of V. It is not a group.

  $\Pi_0(SO(3)) = 0$ 1 component

  $\Pi_0(O(3)) = \mathbb{Z}_2$ 2 components

  $\Pi_0(S^1) = 0$ 1 component

  $\Pi_0(S^0) = \mathbb{Z}_2$ 2 components $S^0 = 2$ points

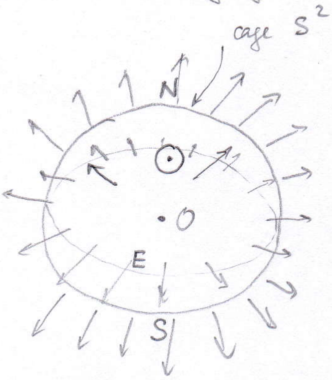
Back to the Heisenberg ferromagnet with $V = S^2$ as $\vec{M}(\vec{r}) \simeq M_0 \vec{n}(\vec{r})$

as $\pi_0(S^2) = 0$ no topological plane-like defect (domain wall)

$\pi_1(S^2) = 0$ ———— line ————

$\pi_2(S^2) = \mathbb{Z}$ topological point-like defects classified by a mapping number. These are known as <u>hedgehogs</u> (and have a close relationship to baby-skyrmions) or <u>Bloch points</u>.

Here is a drawing of the charge +1 hedgehog:



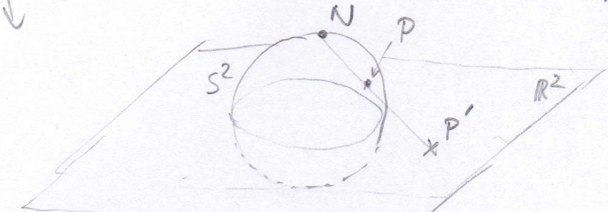
stereographic projection

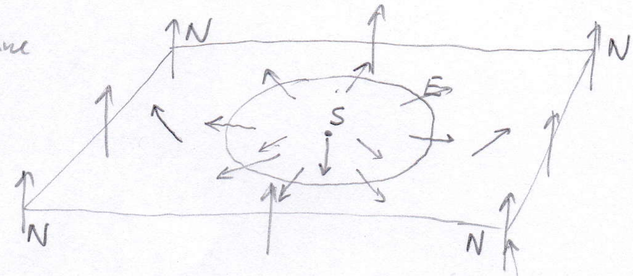
the cage sphere becomes a plane

north pole $\rightarrow \infty$

south pole $\rightarrow$ 0 (origin)

equator $\rightarrow$ equator





cage is now the $\mathbb{R}^2$ plane

do not confuse this with a (baby) skyrmion which is a 2D topological texture and not a 3D topological defect.

remark: domain walls are stable topological textures (solitons, configurations) in 3D Heisenberg ferromagnets. They are not defects (no singularity) and require imposed boundary condition for their existence.

Summary: homotopy groups allow one to think of topological defects

to classify them

to characterize them with integers (known as topological invariants)

stability of topological defects

topological invariants are useful to study the creation / annihilation of topological defects (think of the +1 and −1 vortices of the Kosterlitz-Thouless transition for 2D XY model i.e. $d=2$ and $n=2$).

2) Dirac's magnetic monopole and fiber bundles

Dirac 1931 : electromagnetism and quantum mechanics permit the existence of a quantized magnetic monopole.

Hopf 1931 : Hopf fibration, an example of fiber bundle

a) Quantum mechanics in the presence of a vector potential $\vec{A}$

minimal coupling : $\vec{p} \rightarrow \vec{p} - q\vec{A} = \vec{p} - e\vec{A}$ for a charged particle with electric charge $q = +e$

i.e. $\underset{\text{derivative}}{\vec{\nabla}} \rightarrow \vec{\nabla} - i\frac{e}{\hbar}\underset{\text{connection}}{\vec{A}} \equiv \underset{\text{covariant derivative}}{\vec{D}}$

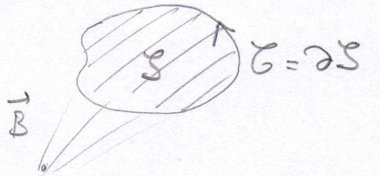
$\vec{B} = \vec{\nabla} \times \vec{A}$ is the curvature

for the wavefunction, it means $\psi(\vec{r}) \longrightarrow \psi(\vec{r})\, e^{+i\frac{e}{\hbar}\int^{\vec{r}} d\vec{\ell}\cdot\vec{A}}$

phase $\theta(\vec{r})$ U(1)

Aharonov-Bohm phase : after parallel transport along a closed path, the wavefunction comes back to itself up to a non-integrable phase (also known as a geometric phase or anholonomy)

$$e^{i\Gamma_{AB}} = e^{i\frac{e}{\hbar}\oint_{\mathcal{C}} d\vec{\ell}\cdot\vec{A}} = e^{i\frac{e}{\hbar}\iint_{S} d^2\vec{S}\cdot\vec{B}} = e^{i\frac{e}{\hbar}\phi}$$ magnetic flux



$\frac{e}{\hbar}\phi$ is a phase, an angle : it matters modulo 2π

$\Rightarrow$ ϕ matters modulo $\frac{h}{e} \equiv \phi_0$: magnetic flux quantum (this is already an addition to Maxwell's electromagnetism)

A gauge transform is a dble transformat°:

. on the vector potential $\vec{A} \longrightarrow \vec{A}' = \vec{A} + \vec{\nabla}\chi$ already in classical electromagnetism (but $\vec{B}$ is unchanged)

. on the wavefunction $\psi(\vec{r}) \rightarrow \psi'(\vec{r}) = \psi(\vec{r})\, e^{i\frac{e}{\hbar}\chi(\vec{r})}$ in QM, $\frac{e}{\hbar}\chi(\vec{r}) = \theta(\vec{r})$

It is a U(1) phase transformation.

b) Magnetic monopole of charge g at $\vec{r}=0$

$$\vec{\nabla}\cdot\vec{B} = g\,\delta(\vec{r}) \quad \text{instead of } 0$$

$$\vec{B} = \frac{g}{4\pi}\frac{\vec{r}}{r^3} \qquad \text{singularity of } \vec{B} \text{ at } \vec{r}=0$$

Is this possible?

What is the flux across a sphere S^2?

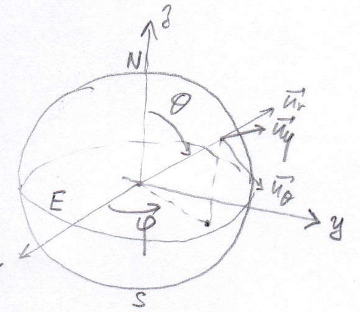
$$\phi = \int_{S^2} d^2\vec{S}\cdot\vec{B} = \int_{\text{Volume}} d^3r\,\underbrace{(\vec{\nabla}\cdot\vec{B})}_{g\,\delta(\vec{r})} = g$$

If there exists a smooth global gauge (i.e. $\vec{A}$ is well defined over all S^2 and such that $\vec{B}=\vec{\nabla}\times\vec{A}$) then Stokes' theorem is applicable and

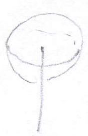
$$\phi = \int_{S^2} d^2\vec{S}\cdot\vec{B} = \int_{S^2} d^2\vec{S}\cdot(\vec{\nabla}\times\vec{A}) = \oint_{\partial S^2} d\vec{\ell}\cdot\vec{A} = 0 \quad \text{as } \partial S^2 = 0.$$

$\Rightarrow$ if $g\neq 0$ then there exist no smooth gauge!

Wu & Yang 1975 introduced the idea of having patches for $\vec{A}$ and a gauge transformation to connect the patches.



North hemisphere:



$$\vec{A}^N = \frac{g}{4\pi}\,\frac{1-\cos\theta}{r\sin\theta}\,\vec{u}_\varphi$$

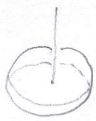
well-defined at N $\quad (\vec{A}^N = 0)$

ill- ——— S $\quad (\vec{A}^S \to \infty)$

$$\to \quad \vec{B}^N = \frac{g}{4\pi}\frac{\vec{u}_r}{r^2} + g\,\delta(x)\,\delta(y)\,\Theta(-z)\,\vec{u}_z$$

$$\vec{\nabla}\cdot\vec{B}^N = 0$$

South hemisphere:



$$\vec{A}^S = \frac{g}{4\pi}\,\frac{-1-\cos\theta}{r\sin\theta}\,\vec{u}_\varphi$$

ill-defined at N

well ——— S

On most of $\mathbb{R}^3$, $\vec{B}^N = \vec{B}^S$; but they disagree along $z<0$ and $z>0$. Therefore, there exist no gauge transformation on all of $\mathbb{R}^3$ that transforms $\vec{A}^N$ into $\vec{A}^S$.

However $\vec{B}^N = \vec{B}^S$ on the equator.

$$\vec{A}^N - \vec{A}^S = \frac{g}{2\pi r\sin\theta}\,\vec{u}_\varphi = \vec{\nabla}\chi \quad \text{with } \chi = \frac{g}{2\pi}\varphi$$

as
$$\vec{\nabla}\chi = \frac{\partial\chi}{\partial r}\vec{u}_r + \frac{1}{r}\frac{\partial\chi}{\partial\theta}\vec{u}_\theta + \frac{1}{r\sin\theta}\frac{\partial\chi}{\partial\varphi}\vec{u}_\varphi$$

The total flux across the sphere is:

$$\phi = \int d^2\vec{S}\cdot\vec{B} = \int_N d^2\vec{S}\cdot(\vec{\nabla}\times\vec{A}^N) + \int_S d^2\vec{S}\cdot(\vec{\nabla}\times\vec{A}^S) = \oint_E d\vec{\ell}\cdot\vec{A}^N - \oint_E d\vec{\ell}\cdot\vec{A}^S$$

$$= \oint_E d\vec{\ell}\cdot\vec{\nabla}\chi = \frac{g}{2\pi}\oint_E d\varphi = g$$

OK. This means that $\vec{\nabla}\cdot\vec{B} = g\,\delta(\vec{r})$ with $\vec{B}$ built from the two patches $\vec{A}^N$ and $\vec{A}^S$.

But χ is also changing the phase of the wf during the gauge transformation:

$$\begin{cases} \vec{A}^S \longrightarrow \vec{A}^N = \vec{A}^S + \vec{\nabla}\chi \\ \psi^S(\vec{r}) \longrightarrow \psi^N(\vec{r}) = \psi^S(\vec{r})\, e^{i\frac{e}{\hbar}\chi(\vec{r})} = \psi^S(\vec{r})\, e^{i\frac{g}{\phi_0}\varphi} \end{cases} \qquad \theta = \pi/2$$

And the wf has to be single-valued ie.

$$\psi^N(r, \theta = \tfrac{\pi}{2}, \varphi + 2\pi) = \psi^N(r, \theta = \tfrac{\pi}{2}, \varphi) \quad \text{and} \quad \psi^S(r, \theta = \tfrac{\pi}{2}, \varphi + 2\pi) = \psi^S(r, \theta = \tfrac{\pi}{2}, \varphi)$$

$$\Rightarrow e^{i\frac{g}{\phi_0}(2\pi + \varphi)} = e^{i\frac{g}{\phi_0}\varphi} \quad \text{ie.} \quad e^{i 2\pi \frac{g}{\phi_0}} = 1$$

$$\boxed{g = \text{integer} \times \phi_0}$$

A magnetic monopole is possible but its charge should be quantized.
The wavefunction along the equator is actually a wave-section.

remark: • a <u>non-zero monopole charge</u> can be seen as <u>an obstruction to finding a smooth global gauge</u>.

• total flux across the sphere

$$\frac{\phi}{\phi_0} = \frac{1}{\phi_0} \int_{S^2} d^2\vec{S} \cdot \vec{B} = \frac{g}{\phi_0} = \text{integer} \in \mathbb{Z}$$

if ϕ matters modulo ϕ_0 then a quantized magnetic monopole is the modulo

These two features will be encountered later when discussing Chern numbers.

Rk: $\vec{A}$ is more fundamental than $\vec{B}$ even if $\vec{A}$ is gauge-dependent and $\vec{B}$ is gauge-invariant.

c) <u>The Wu & Yang dictionary: from gauge fields to fiber bundles</u>

There is a mathematical (geometrical) notion hidden here. It is that of fiber bundles.
Wu & Yang 1975 understood that gauge fields (in physics) = fiber bundles (in maths).

after the Möbius strip.

electromagnetism	fiber bundle (a U(1) complex vector bundle)
$\vec{A}$ vector potential	connection (describes parallel transport)
$\vec{B}$ magnetic field	curvature
Γ_{AB} AB phase	anholonomy (in parallel transport) geometric phase
Dirac's monopole quantization	classification of U(1) bundles according to the 1st Chern number
$-i\hbar\vec{\nabla} - e\vec{A}$ minimal coupling	covariant derivative
$\psi^N(\vec{r}) = \psi^S(\vec{r})\, e^{i\frac{g}{\phi_0}\varphi}$ wavefunction on the equator region; integer	section (rather than a function)

Fiber bundle is a notion of geometry (~ Whitney 1930's)

a fiber bundle E ~~compact~~

consists of a base space B (a manifold) e.g. S^1

and of a fiber F e.g. $\mathbb{R}$ or a segment $[0,1]$ or S^1

a projection map $p: \quad E \longrightarrow B$

$$F \hookrightarrow E \xrightarrow{p} B$$

$\boxed{\text{locally } E \text{ looks like } B\times F \text{ but not necessarily globally}}$

a structure group G can act on the fiber (e.g. $G=U(1)$ if $F=S^1$)

if globally $E=B\times F$ the bundle is said to be trivial

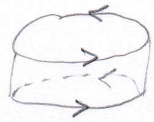
if ~~locally~~ $E\neq B\times F$ ——————— twisted or non-trivial.

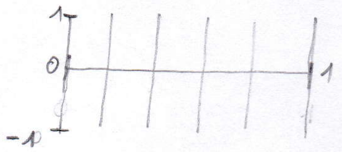
A twisted fiber bundle is characterized by topological invariants (called characteristic classes). The most famous is the Chern number.

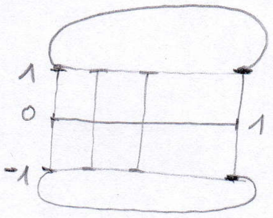
ex: Möbius strip (Möbius ; Listing 1858)

$B=S^1$ (first $[0,2\pi]$ and then S^1)

$F=[-1,1]$ and then S^1



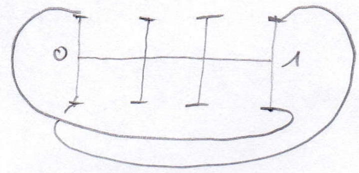




cylinder

$E=B\times F$

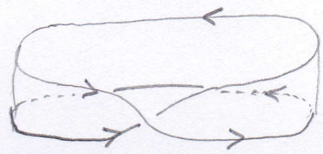
trivial bundle



Möbius strip

twisted bundle

$E\neq B\times F$



a single edge and

a single side

(non-orientable)

other similar example is the Klein bottle VS the torus with $B=S^1$ and $F=S^1$

$\uparrow$

$T^2=S^1\times S^1$

Back to the Dirac monopole :

Hopf bundle, fibration

$B=S^2$ (as $\mathbb{R}^3\setminus\{0\} = S^2\times\mathbb{R}^{+*} \sim S^2$)

$F=S^1$ (is the phase) $S^1\hookrightarrow E \xrightarrow{p} S^2$

$G=U(1)$ (is the gauge freedom) S^3

$$S^1 \hookrightarrow \underset{\underset{S^3}{\parallel}}{E} \xrightarrow{p} S^2$$

Is this bundle twisted ?

- No global section i.e. obstruction
- The answer is contained in the Chern number :

(This is also the charge of the monopole)

$$C=\frac{1}{\phi_0}\int_{S^2} d^2\vec{S}\cdot\underset{\underset{\text{curvature}}{\uparrow}}{\vec{B}} = \frac{g}{\phi_0} = \text{integer} \neq 0$$

i.e. $\vec{B}=\dfrac{C}{2}\dfrac{\vec{r}}{r^3}$

remark: this is not the same as a point-like topological defect in a 3D superfluid for which $d=3$, $n=2$, $V=S^1$ and

$$\Pi_2(S^1)=0$$

Hopf invariant classifies maps $S^3\rightarrow S^2$

$$\Pi_3(S^2)=\mathbb{Z}$$